

ATOMISTIC COHESIVE ZONE MODELS FOR INTERFACE DECOHESION IN METALS

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ABSTRACT Using a statistical mechanics approach, a cohesive-zone law in the form of a traction-displacement constitutive relationship characterizing the load transfer across the plane of a growing edge crack is extracted from atomistic simulations for use within a continuum finite element model. The methodology for the atomistic derivation of a cohesive-zone law is presented. This procedure can be implemented to build cohesive-zone finite element models for simulating fracture in nanocrystalline or ultrafine grained materials.

INTRODUCTION: Cohesive zone models (CZMs) can be developed to represent constitutive relations for crack propagation along an interface. They are frequently used in conjunction with the finite element method to study fracture in a wide variety of materials. When derived empirically at macroscopic length scales, the peak traction and maximum opening displacement in these models represent the aggregate responses of thousands or millions of grains, grain boundaries, and defects within the specimens from which they were obtained. At this length scale, the unique response of a particular microstructural interface at which a local fracture event might occur cannot be represented. If microscale predictions are of interest, consideration of the local nanoscale properties is required. At the nanoscale, a CZM is an integrated description of the atomic debonding processes and is dependent upon the interatomic forces in the material.

This paper will review existing methodologies for extracting CZMs from atomistic simulations. The main goal of these methodologies is to extract and understand the contributions of different atomistic processes to an atomistic-based CZM decohesion law for interface debonding in ductile metals, such as aluminum. A newly developed and successfully implemented approach will be presented. The approach is based on a statistical mechanics derivation of a CZM law from a multimillion atom, molecular dynamics (MD) simulation of crack propagation under steady-state conditions. The derived CZM law can be incorporated into a finite element model for use in continuum mechanics models of crack propagation.

PROCEDURES, RESULTS AND DISCUSSION: In this study, CZM laws are developed using the tractions and displacements obtained along a crack path within coupled atomistic-continuum models. The coupled models allow a large atomistic domain (containing 10^6 or more atoms) to be embedded within a continuum domain of

micron dimensions. The atomistic domain is simulated using molecular dynamics, where the interatomic forces are represented by an atomistic potential suitably fitted to reproduce the material properties of aluminum (Mishin et al. 1999). The continuum domain is simulated by using the finite element method (FEM) with anisotropic elastic properties derived from the aluminum potential at room temperature (300K). The coupling between FEM and MD is achieved by the recently developed embedded statistical coupling method (ESCM) (Saether et al. 2007) to provide elastic boundary conditions for the atomistic domain and transfer the applied far field mechanical load into the atomistic system. In the present study, the method is used to simulate an edge crack in a square aluminum plate of 0.9 μm size and a thickness of 3 to 25 nm. The embedded MD region is formed as a circle of 40 nm diameter around the crack tip in the middle of the square plate. A uniaxial tensile strain from 0.1% to 1.5% is applied to the system. The resulting mode I stress intensity at the crack tip is from 0.05 to 0.77 $\text{MPa}\cdot\text{m}^{1/2}$. Periodic boundary conditions along the thickness direction were used in the atomistic region equivalent to plane strain conditions in the continuum region. Under these conditions, a steady-state crack propagation has been achieved in the atomistic region.

To extract the CZM constitutive relation, atomic volumes called cohesive-zone-volume-elements (CZVEs), were defined along the crack path in the atomistic region of the model (Fig. 1). Each CZVE is of nanometer size dimensions, containing a statistically large number of atoms (a few hundred to a few thousand atoms per CZVE). The state of each CZVE at position x and instant of time t is defined by the state variables $\sigma_{yy}(x,t)$ and $\lambda(x,t)$. At a given time t , $\sigma_{yy}(x,t)$ and $\lambda(x,t)$ present the stress and opening displacement profiles along the crack plane, as shown in Fig. 1. The CZVE state is represented as a point in a σ_{yy} - λ configuration space (Fig. 2). In the statistical limit of steady-state crack propagation that occurs over an infinitely long time over an infinitely long interface, all realized CZVE states would produce a distribution, $\rho(\lambda, \sigma_{yy})$, (density of states) that is a continuous function independent of time. The CZM is defined as a statistical average, $\bar{\sigma}_{yy}(\lambda)$, of σ_{yy} over a small interval $(\lambda - \Delta\lambda, \lambda + \Delta\lambda)$ of this distribution at the limit of $\Delta\lambda \rightarrow 0$

$$\bar{\sigma}_{yy}(\lambda) = \langle \sigma_{yy}(\lambda) \rangle = \frac{\int_{\lambda'=\lambda-\Delta\lambda}^{\lambda+\Delta\lambda} \int_{\sigma'_{yy}=-\infty}^{\infty} \sigma'_{yy}(\lambda') \rho(\lambda', \sigma'_{yy}) d\sigma'_{yy} d\lambda'}{\int_{\lambda'=\lambda-\Delta\lambda}^{\lambda+\Delta\lambda} \int_{\sigma'_{yy}=-\infty}^{\infty} \rho(\lambda', \sigma'_{yy}) d\sigma'_{yy} d\lambda'} . \quad (1)$$

Numerically, $\rho(\lambda, \sigma_{yy})$ can be approximated by using the previously described coupled MD-FEM simulation model. For a finite number of measurements, $\rho(\lambda, \sigma_{yy})$ takes a discrete form $\rho(\lambda, \sigma_{yy}) = \sum_i \delta(\lambda - \lambda_i) \delta(\sigma_{yy} - \sigma_{yy}(\lambda_i))$, where the sum is over all measured data points $(\lambda_i, \sigma_{yy}(\lambda_i))$ and $\delta(x - x_i)$ is the Dirac delta function. The discretization of Eq. (1) takes the form of a moving average

$$\bar{\sigma}_{yy}(\lambda) = \langle \sigma_{yy}(\lambda) \rangle = \frac{1}{N(\lambda_i \in \{\lambda - \Delta\lambda, \lambda + \Delta\lambda\})} \sum_{i=1}^N \sigma_{yy}(\lambda_i), \quad (2)$$

where the sum is taken over all N points (λ, σ_{yy}) , which are between $\lambda - \Delta\lambda$ and $\lambda + \Delta\lambda$. The choice of the size of the interval, $\Delta\lambda$, depends on the desired resolution of the CZM with respect to λ .

Figure 2 shows the derived $\rho(\lambda, \sigma_{yy})$ distribution for the example given in Fig. 1, after collecting data from 180 snapshots that were taken at intervals of 1 ps. The averaged stress-displacement curve $\bar{\sigma}_{yy}(\lambda)$ is closely approximated by a least-square bilinear fit to the extracted $\rho(\lambda, \sigma_{yy})$ distribution, which is more computationally efficient to use as a CZM law in FEM models. The two points, (λ_p, σ_p) and $(\lambda_0, 0)$ were used as fitting parameters (Fig. 2). The CZM law derived by this technique is free of finite size effects and is statistically representative for describing the interfacial debonding of an idealized material interface examined at atomic length scales.

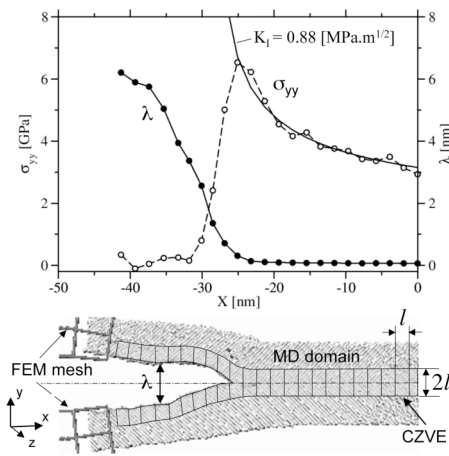


Fig.1 Stress and opening profiles from CZVEs along an edge crack.

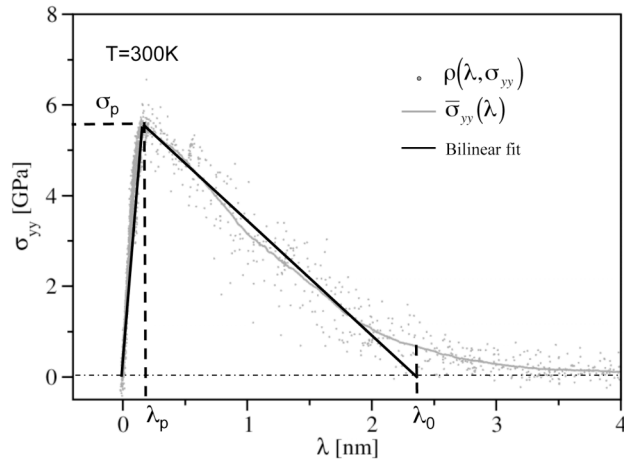


Fig.2 Bilinear CZM, parameterized as a least-square fit to the extracted statistical stress-displacement distribution

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REFERENCES:

- Mishin Y., Farkas D., Mehl M. J., Papaconstantopoulos D. A., 1999, "Interatomic Potentials for Monoatomic Metals from Experimental Data and ab initio Calculations," Phys. Rev. B, **59** 3393-3407.
- Saether E., Yamakov V., Glaessgen E., 2007, "A Statistical Approach for the Concurrent Coupling of Molecular Dynamics and Finite Element Methods," 49th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference.